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LETTER TO THE EDITOR

Critical comparison between theory and experiment for C^{6+}+He fully differential ionization cross sections

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Abstract
Fully differential cross sections for single ionization of helium induced by impact of 100 MeV/u C^{6+} ions are examined within a quantum-mechanical distorted wave model. The experimental uncertainties are included in the theoretical calculations, leading to a quantitative description of the experimental cross sections. In particular, the ionization cross section for the electron emitted in the plane perpendicular to the scattering plane is reproduced for the first time by a full quantum-mechanical model. The role of the internuclear interaction in this perturbative-regime collision is discussed and found to be unimportant for the present kinematical conditions.

(Some figures in this article are in colour only in the electronic version)

In a recent series of publications, serious discrepancies between quantum mechanically calculated continuum distorted wave (CDW) fully differential cross sections (FDCS) and measurements were discussed (Fischer *et al* 2003a, Fainstein and Gulyás 2005, Fiol and Olson 2003, Rodríguez 2003, Madison *et al* 2003, Schulz *et al* 2003a). In particular, the C^{6+}+He system was very puzzling. At 100 MeV/u, where the Sommerfeld parameter measured by the projectile charge to velocity ratio is $Z/v = 0.10$, a comparison between calculations and observations revealed a total lack of agreement for scattering perpendicular to the collision plane (Schulz *et al* 2003a). In fact, the calculations predicted slight minima in the cross sections at 90° and 270°, while the experiments exhibited strong maxima with cross section absolute magnitudes approximately four times larger than the calculations. Further studies on this system, but at 2 MeV/u where the Sommerfeld parameter increases to $Z/v = 0.67$, again indicated serious discrepancies between theory and experiment (Madison *et al* 2003), particularly in the plane perpendicular to that of the collision. The conclusions of the latter paper indicated that there is a failure in the CDW method for the range of impact parameters probed by the experiments. Thus, one is led to conclude that state-of-the-art quantum mechanical calculations exhibit fundamental flaws when tested at the fully differential (kinematically complete) level.

In a recent letter, we showed that these observed fully differential cross sections are extremely sensitive to momentum uncertainties. Classical trajectory Monte Carlo (CTMC) calculations for the highly non-perturbative 3.6 MeV/u Au^{53+} + He system, $Z/v = 4.4$, demonstrated that the fully differential cross sections vary up to two orders-of-magnitude, and their angular dependencies change dramatically by including small uncertainties in the experimental momenta (Olson and Fiol 2005). Important changes were also observed concerning the intensity of the forward electron emission when momentum uncertainties were taken into account for the C^{6+}+He system at 2 MeV/u (Otranto *et al* 2006).

In this letter, we have utilized a computer intensive method that incorporates the published momentum uncertainties within the quantum mechanical CDW method in order to make quantitative comparisons with experiment. These experimental uncertainties are available in publications concerning the C^{6+}+He measurements (Fischer *et al* 2003a, 2003b, Schulz *et al* 2004). We find that by including the experimental uncertainties most of the discrepancies between experiment and theory are removed. In fact, the conclusions regarding the inadequacy of CDW calculations are not supported if the experimental data are analysed in detail.

In this work we analyse the cross section $\mathrm{d}\sigma/\mathrm{d}E_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{e}\,\mathrm{d}\Omega_\mathrm{P}$ differential in the projectile scattering angle, electron energy and angles. We employ a quantum-mechanical CDW three-body model that includes the internuclear (NN) interaction on the same level of approximation as the interactions of the electron with the projectile and with the residual-target-ion (Fiol *et al* 2001, Fiol and Olson 2003, and references therein). The He^+ residual-ion has been modelled as a single-particle with an effective interaction given by a central two-parameter potential based on Hartree–Fock calculations (Garvey *et al* 1975). The same model potential has been used for the initial and final electron-target states as well as for the internuclear perturbation. Relativistic effects are only included in the incident velocity of the projectile, while the treatment of all interactions is non-relativistic.

In order to quantitatively compare with the measured cross sections we must include the experimental uncertainties. We have convoluted the theoretical FDCS with the momentum distributions following the reported uncertainties (Fischer *et al* 2003a, 2003b, Schulz *et al* 2004, Moshammer *et al* 1996). The inclusion of the uncertainties of the experiment has been carried out by integrating the calculated cross sections over the vector momentum transfer $\boldsymbol{Q}$ weighted by a Gaussian distribution. This convolution requires considerable computational effort; in this work over 600 cross sections are calculated in order to get each averaged value of the FDCS. In total, more than 6×10^4 FDCS calculations were needed for the convolutions.

The most puzzling results in relation with ionization by fast heavy ions were the reported comparisons between theory and experiment for helium ionization by impact of 100 MeV/u C^{6+}. For electrons emitted in the plane perpendicular to the momentum transfer $\boldsymbol{Q}$ that contains the incident velocity $\boldsymbol{v}$ (which will be referred as the perpendicular plane) strong disagreement between experiment and theory is observed both in shape and magnitude.

Due to the large impact velocity of the projectile, the cross sections involved are very small and experiments are difficult to perform. On the other hand, besides possible relativistic effects, the quantum-mechanical description of such processes is expected to be well followed by simple perturbative methods. In particular, a first-order Born approximation (FBA) was believed to be correct at such high incident velocity (Bates and Griffing 1953). However, recent publications have concluded that this is not the case, and that even state-of-the-art CDW approximations (CDW-EIS and 3DW models) are unable to describe the measured FDCS. It has also been suggested that the discrepancies were related to the inadequateness

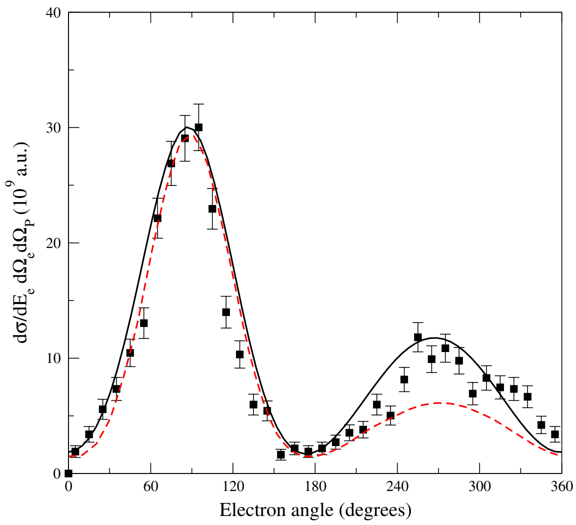

Figure 1. Fully differential cross section for single ionization of helium by 100 MeV/u C^{6+}. The electrons are emitted in the scattering plane with energy $E_e = 6.5$ eV. The momentum transfer is $Q = 0.75$ au. Solid symbols are experimental results by (Schulz *et al* 2003a); dashed line: CDW model; solid line: CDW model convoluted over the experimental uncertainties.

of the CDW wavefunction close to the origin (Madison *et al* 2002, 2003). Figure 1 presents the fully differential cross sections for ionization of helium where the electrons are emitted in the projectile scattering plane, containing the initial velocity and the momentum transfer vectors. The electrons are emitted with an energy 6.5 eV. The magnitude of the momentum transferred by the projectile to the target system is $Q = 0.75$ au, which corresponds to a laboratory scattering angle $\theta_P \approx 6 \times 10^{-4}$ mrad.

In contrast to what has been previously reported, the theoretical values agree well (solid curve) with the experiment in both shape and absolute magnitude once the experimental uncertainties are convoluted into the theory. We note that the experimental data have been normalized to FBA calculations (Schulz *et al* 2003a). The dominant structure at $\theta \approx 90°$, the binary peak, is well described by first-order theories and does not change appreciably by including the target momentum experimental uncertainty. Only for electron emission angles close to 270°, the recoil peak, do the CDW cross sections differ considerably from the measured values. As seen, the convolution with the experimental uncertainties increases the value of the recoil maximum by a factor of two compared to that without such a convolution.

The reason for this important increase of the recoil peak after the convolution is related mainly to the inclusion of cross sections corresponding to smaller momentum transfers Q. Not only do the absolute values of the cross sections increase with decreasing momentum transfer, but also the ratio recoil-to-binary peak increases proportionally, as shown in figure 2.

When the uncertainties are taken into account, even more dramatic modifications are observed in the FDCS for electrons emitted in the perpendicular plane. As shown in figure 3, the curve for the convoluted cross sections agrees nearly perfectly with the experimental data both in magnitude and shape. Observe that the curves must be symmetric around $\theta = 180°$, a condition that is fulfilled by the experiment within the published errors. Also, as can be seen from figures 1 and 3, the calculated cross section in the scattering plane is much larger than

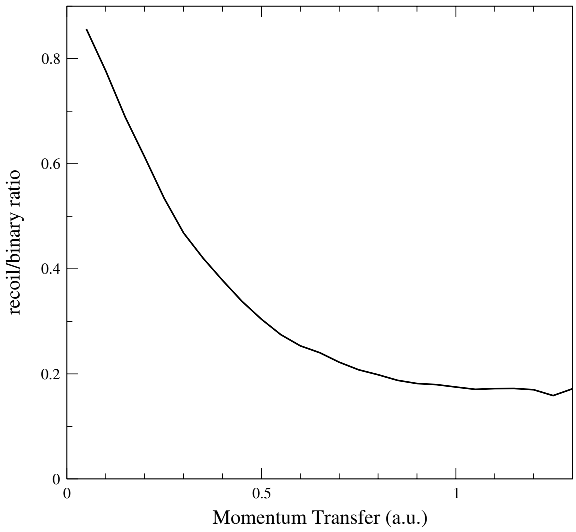

Figure 2. Ratio of theoretical recoil ($\theta = 270^\circ$) to binary ($\theta = 90^\circ$) peak in the FDCS for single ionization of helium by 100 MeV/u C^{6+} as a function of the momentum transfer Q.

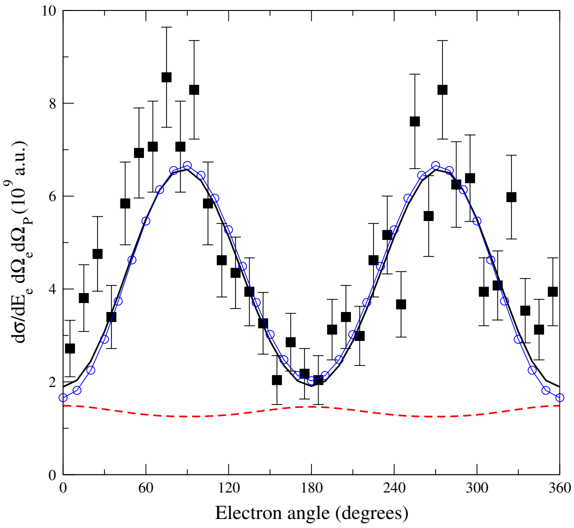

Figure 3. Fully differential cross section for single ionization of helium by 100 MeV/u C^{6+}. The electrons are emitted in the perpendicular plane, defined by the incident velocity and the momentum transfer vector. The momentum transfer is $Q = 0.75$ au and the electron energy is $E_e = 6.5$ eV. Solid symbols are experimental results by (Schulz *et al* 2003a); dashed line: CDW model; solid line and line with open circles are respectively CDW and FBA models convoluted over the experimental uncertainties.

in the perpendicular plane. Thus, by including the uncertainties, both the region from small momentum transfer and a portion of the scattering plane contributes to the observed FDCS in the perpendicular plane.

In contrast to a recent publication (Schulz *et al* 2003b), we note that the internuclear (NN) interaction does not play a significant role for this system in the present conditions. In figure 3

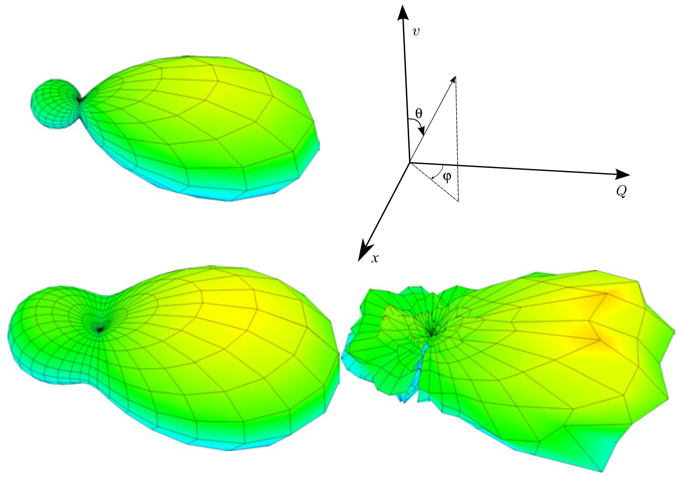

Figure 4. Three-dimensional plot of the fully differential cross section for single ionization of helium by 100 MeV/u C^{6+} for $Q = 0.75$ au and $E_e = 6.5$ eV. Top left: CDW model results neglecting the target momentum uncertainties. Bottom left: CDW model convolved over the experimental resolution. Bottom right: experimental data from Schulz *et al* (2003a). The scattering plane is defined in these plots by the vectors $\boldsymbol{v}$ and $\boldsymbol{Q}$ while the perpendicular plane is defined by the vectors $\boldsymbol{v}$ and $\boldsymbol{x}$.

we also show ionization cross sections in the perpendicular plane calculated within a simple FBA with the same description of the target initial and final states for the active electron as was used for the CDW theory.

A third demonstration of how including the experimental uncertainties modifies the theoretical results is shown in the three-dimensional plots of the FDCS in figure 4. Here the inclusion of the experimental uncertainties not only modifies the magnitude of the cross sections, but the overall shapes are dramatically changed. The well-known double-lobe structure, observed previously for this system (Olson and Fiol 2003) is converted, after convolution, to an 'eye' structure near the origin very similar to the one observed in the experiment (Schulz *et al* 2003a).

Decades of work imply that for a collision system in the perturbative regime ($Z/v = 0.10$) the FBA should describe the experimental data. For this reason, FBA calculations were performed. We obtain very good agreement with the data provided we include the experimental conditions. We note also that the three-dimensional plots with the convolved cross sections calculated with the FBA (not shown here) are almost identical to those obtained with the CDW model.

Summarizing, we have presented quantum-mechanical single-ionization fully differential cross sections for the 100 MeV/u C^{6+}+He collision system. Previous results for this system have led to puzzling conclusions regarding the adequacy of perturbative models to describe the experimental results (Madison *et al* 2002, 2003, Schulz *et al* 2003a). In particular, measured FDCS in the plane perpendicular to the scattering plane that contains the incident velocity presents a maximum at 90° that was not reproduced by previous quantum mechanical theoretical calculations. In this work by taking into account the experimental conditions we have shown that those conclusions are not supported. In fact, not only do state-of-the-art CDW calculations nicely fit the measured data, but also a much simpler FBA gives a very similar description. These latter results allow us to conclude that the internuclear interaction does not play a significant role in the observed cross sections, in disagreement with work that concludes that a higher-order theory is needed (Madison *et al* 2002, 2003, Schulz *et al* 2003a). Our conclusions hold for the chosen kinematical conditions, but it is expected that in the general case both the internuclear interaction and higher-order terms of the projectile-electron interaction will be important. The present findings reinforce previous conclusions that comparison between theoretical models and experiment for FDCS in ion–atom collisions must include an accurate description of experimental uncertainties (Olson and Fiol 2005, Otranto *et al* 2006).

Acknowledgments

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